Projecting Ice Sheet and Climate Evolution at Extreme Scales (PISCEES)

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U.S. DEPARTMENT OF ENERGY Office of Science

SciDAC Scientific Discovery through Advanced Computing

Motivation and Overview

Focus Area Updates

Science Applications

Summary

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Motivation

Ice Sheets and Sea Level Rise

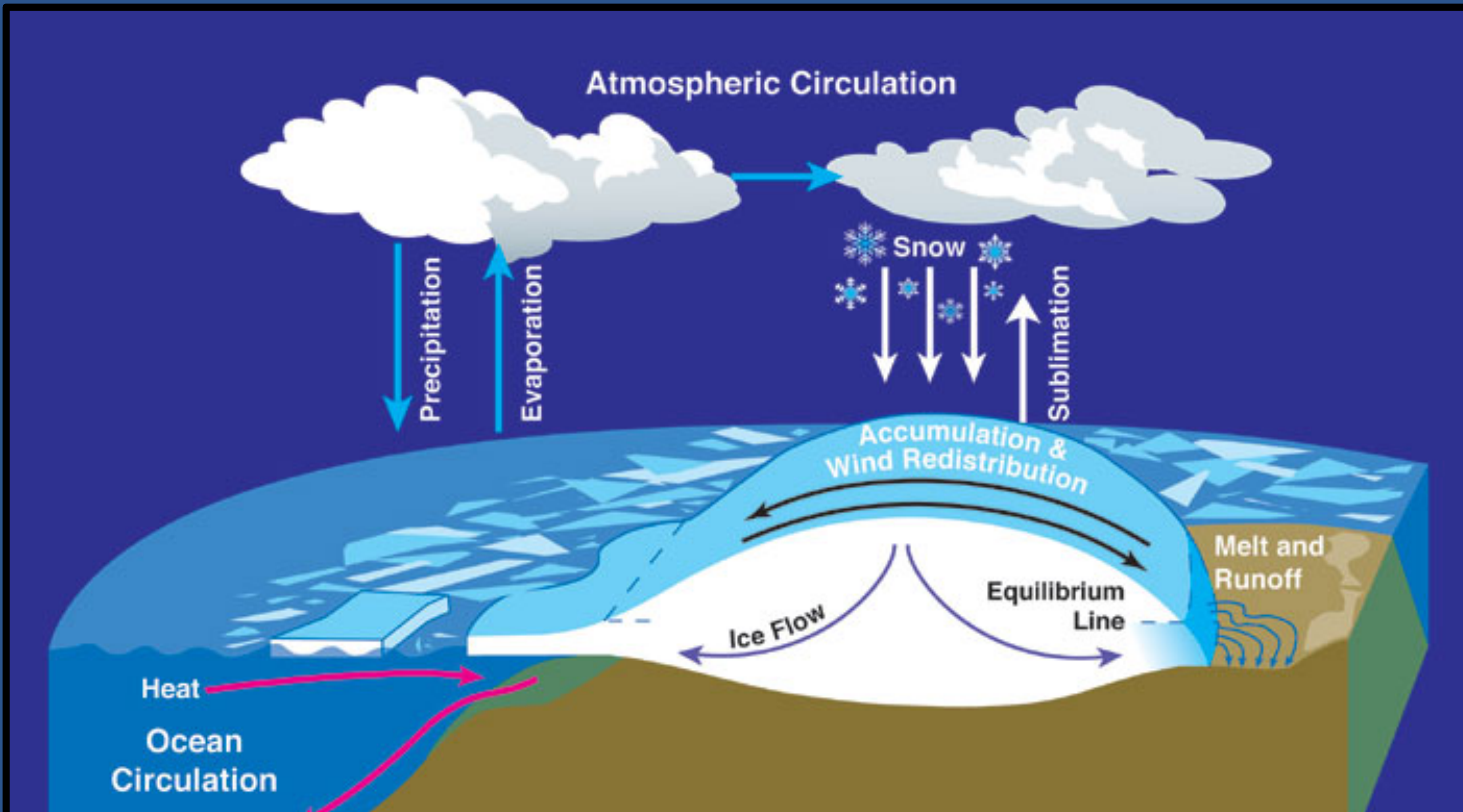
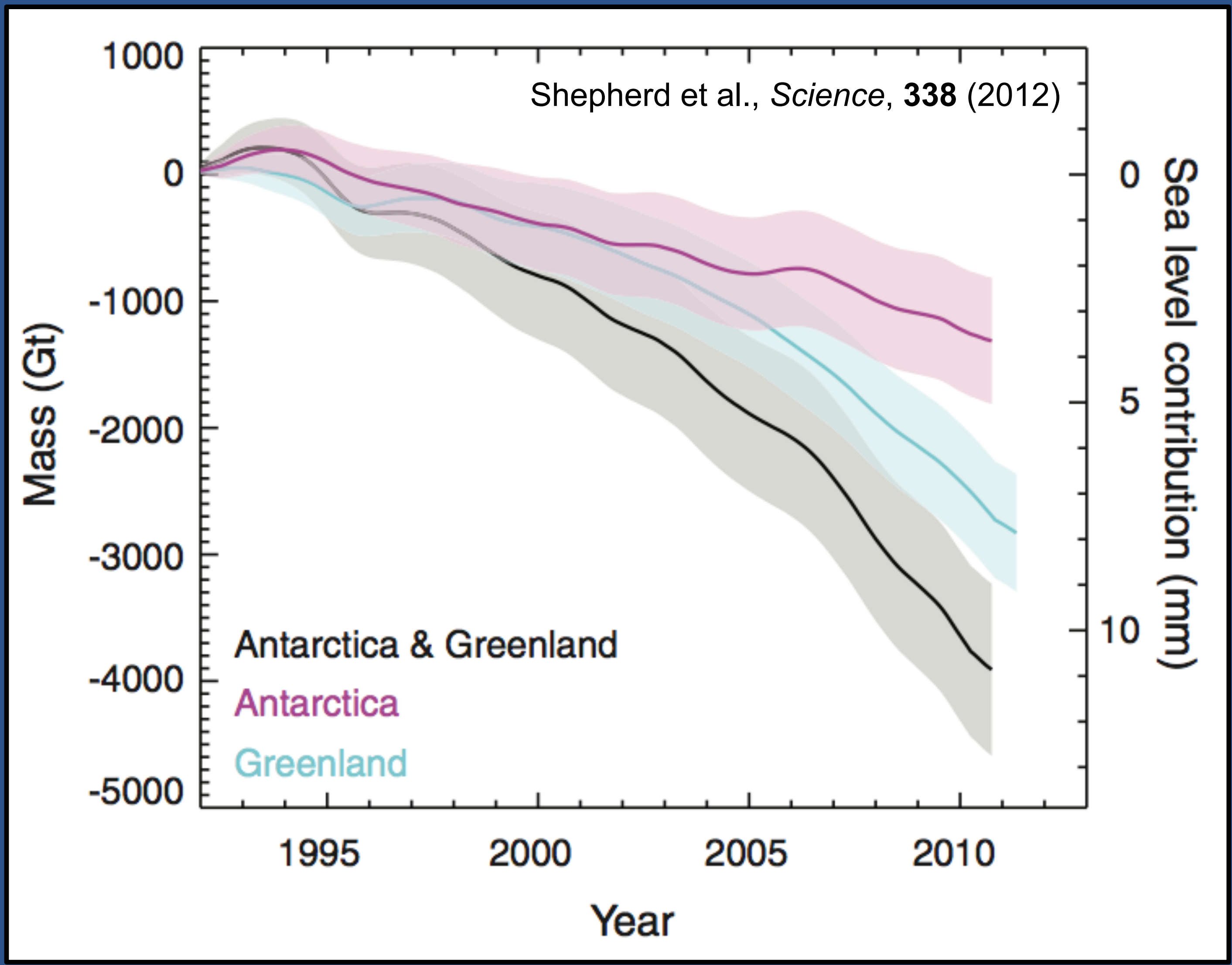


Image source: http://www.nasa.gov/images/content/53743main_atmos_circ.jpg

Mass Balance: Change in ice sheet mass = mass in – mass out
sea level change *snowfall* *melt, calving*

Motivation

Mass loss from the Greenland & Antarctic ice sheets is accelerating.



Project Overview

Mission Statement: Mass loss from the Greenland and Antarctic ice sheets is accelerating. Although ice sheet models have improved in recent years, much work is needed to make these models robust and efficient on continental scales and to quantify uncertainties in their projected outputs.

PISCEES aims to :

1) develop / apply robust, accurate, scalable dynamical cores (dycores) for ice sheet modeling on structured and unstructured meshes with adaptive refinements **(FASTMath; SUPER)**

2) evaluate models using new tools and data sets for verification and validation and uncertainty quantification **(SDAV; QUEST)**

3) Integrate models / tools into DOE-supported Earth System Models

Project Overview

PISCEES builds on past BER / ASCR investments:

- **SciDAC2:** initial coupling of Glimmer ice sheet model to CESM
- **IMPACTS:** coupling between ice sheets and ocean circ. models; simulations of Antarctic ice sheet & ocean coupled evolution
- **ISICLES:** addition of scalable parallelism & interface to FASTMath libraries in CISM; initial devel. of next gen. dycores (continued under PISCEES)

Project Overview

PISCEES is transitioning from development mode to support for science:

1) projections of future SLR from the Antarctica ice sheet

2) quantifying uncertainty in projections of future SLR from ice sheets

Motivation and Overview

Focus Area Updates

- Dynamical cores
- Verification and Validation
- Coupling to Earth System Models (ESM)
- Uncertainty Quantification (UQ)

Summary

Motivation and Overview

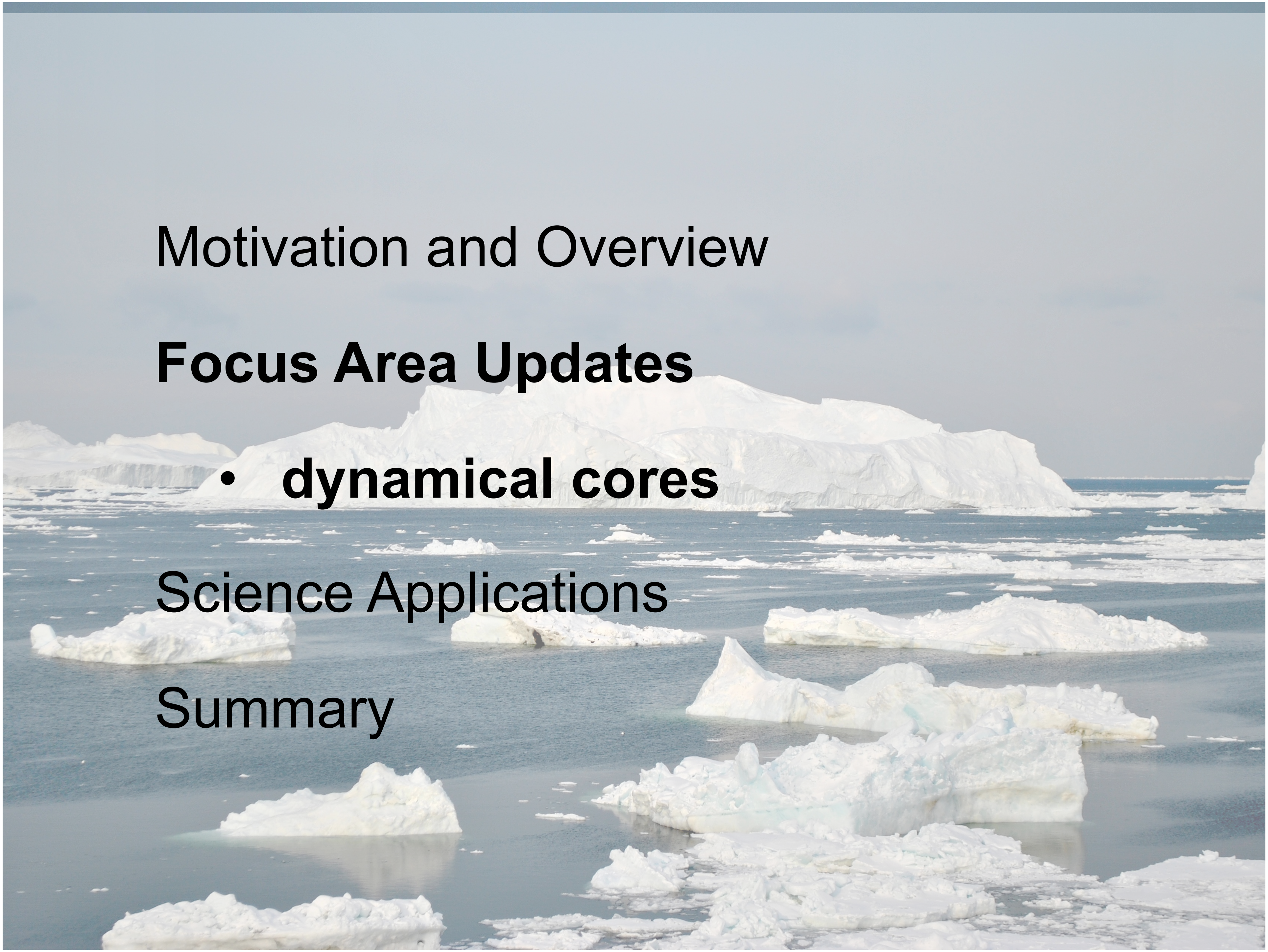
Focus Area Updates

- Dynamical cores
- Verification and Validation

Science Applications

- future SLR from Antarctica (ESM)
- uncertainty in future SLR from ice sheets (UQ)

Summary



Motivation and Overview

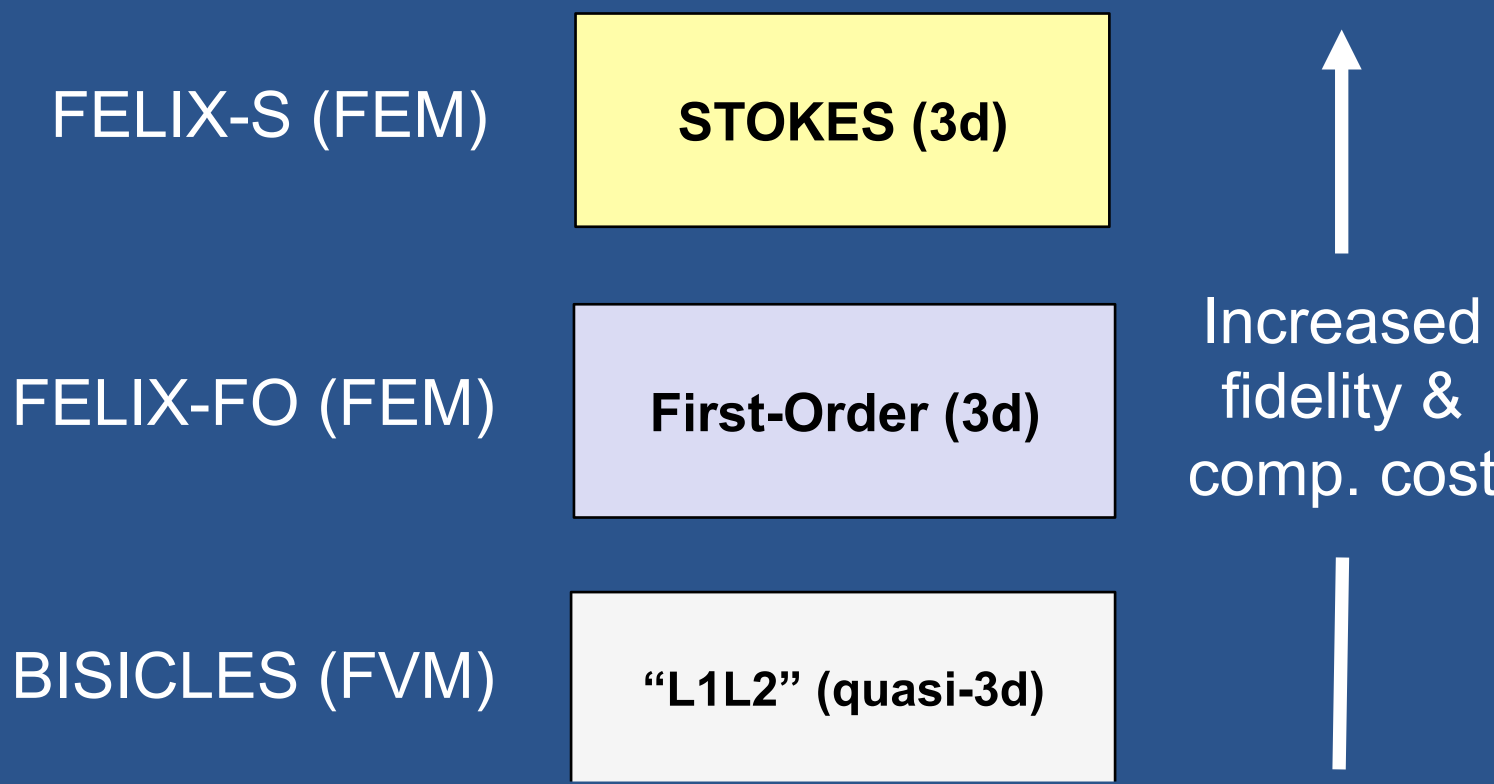
Focus Area Updates

- **dynamical cores**

Science Applications

Summary

Dynamical Core Development



Status:

- range of models & approaches needed (considerations: data resolution, BCs, accuracy vs. cost, etc.)
- comparisons using idealized & limited domain test cases to indicate which appropriate for particular situation
- model down select ("bake off") would be premature at this time

Dynamical Core Development

<u>Land Ice Modeling Framework #1</u>

Community Ice Sheet Model: CISM

- regular, structured grid
- mature, fully-functioning ice sheet model
- coupled to BISICLES and FELIX-FO under PISCEES
- coupled to CESM (& ACME v.0)

<u>Land Ice Modeling Framework #2</u>

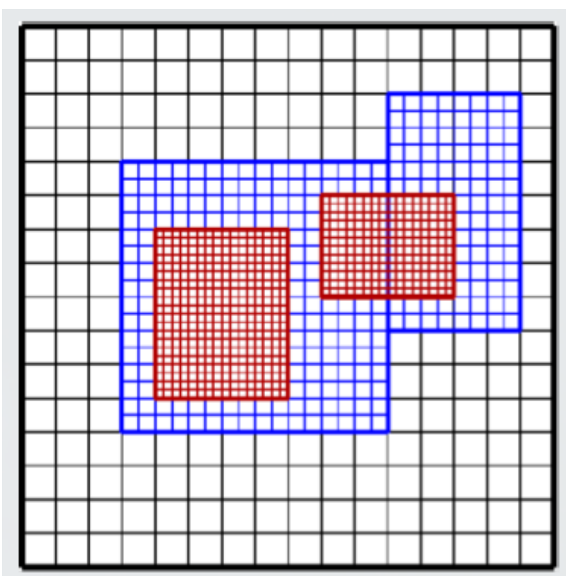
Model for Prediction Across Scales: MPAS-Land Ice

- unstructured, variable resolution, Centroidal Voronoi Tesselations
- under active development, rapidly maturing
- coupled to FELIX under PISCEES
- currently being coupled to ACME

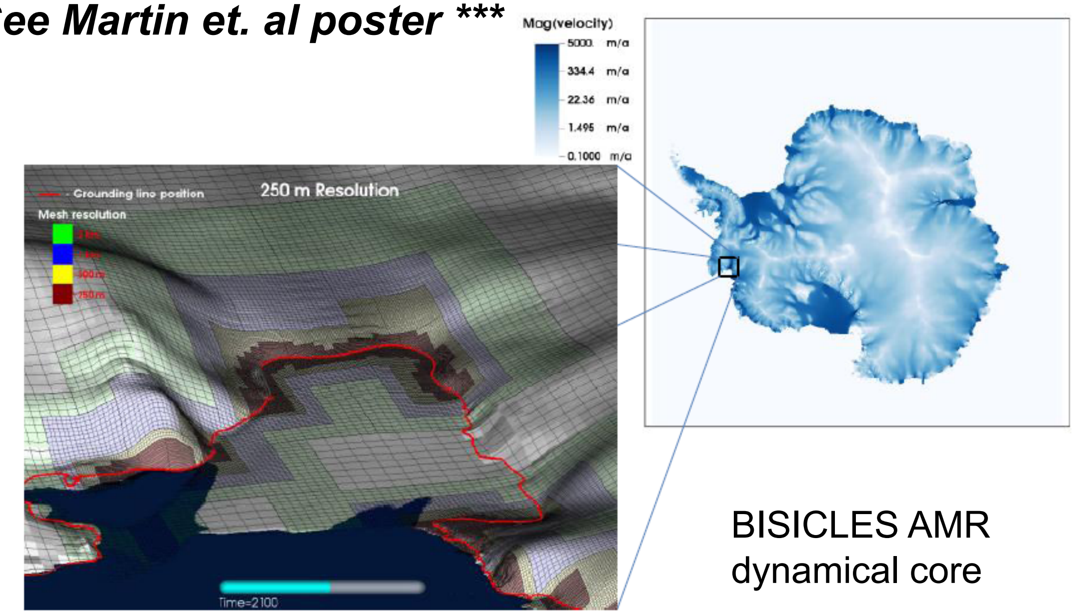
BISICLES Dynamical Core

- "L1L2" momentum balance - formally 1st-order Stokes approx.[2]
- Block-Structured, *dynamic* AMR (for accuracy in dyn. complex regions)
- FVM, built using FASTMath libraries: *Chombo* + *PETSc* AMG
- Performance metrics and tuning through SUPER
- Marine ice sheet dynamics - similar to high-resolution Stokes [3,4]
- Optimization of sliding param. & ice softness to match obs. vels.
- Coupled to Community Ice Sheet Model (CISM); Plans for coupling to ACME

block structured AMR



****** See Martin et. al poster ******



BISICLES AMR dynamical core

[1]Cornford et al. (2012); [2]Schoof and Hindmarsh (2010); [3]Pattyn et al. (2013); [4]Pattyn & Durand (2013)

FELIX Dynamical Cores

FELIX-FO [1]

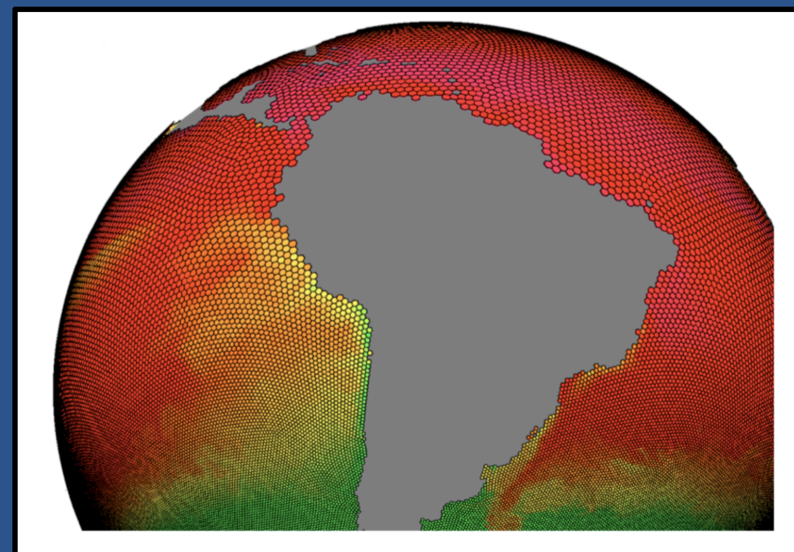
3d, first-order accurate Stokes approx.

FEM using struct. or unstruct. hex. and tet. elements of variable order

Built using FASTMath libraries: *Trilinos* + *Albany*

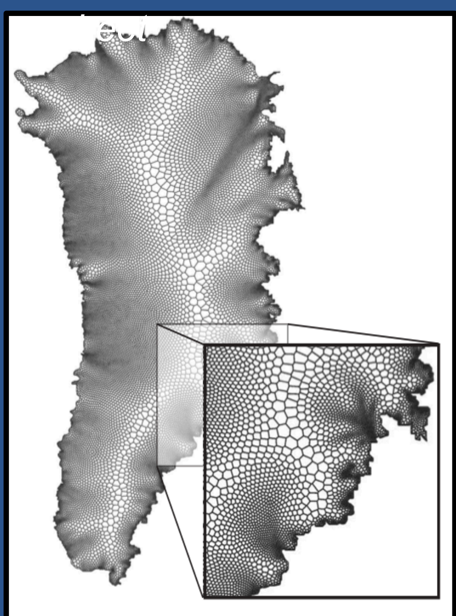
Performance metrics and tuning through SUPER

Coupled to CISM and MPAS-LI



global, variable resolution ocean SCVT

variable resolution CVT of Greenland ice



FELIX-S [2]

Nonlinear ("full") Stokes momentum balance

FEM tet. enhanced Taylor-Hood (P1-P2) elements

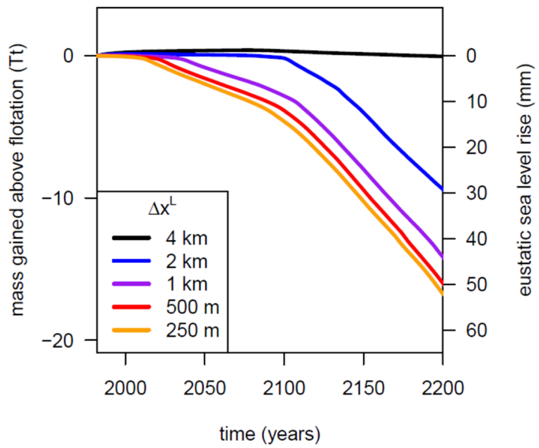
Built using FASTMath libraries: *PETSc*

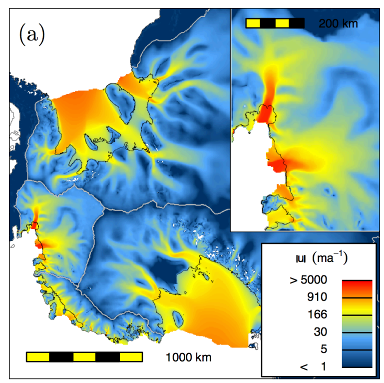
Coupled to MPAS-LI

****** See Tezaur et. al poster ******

[1] Tezaur et al. (2015a, 2015b) [2]Leng et al. (2012a; 2012b; 2014)

Dycore Publications





Cornford, Martin et al., *The Cryos.* (2015)

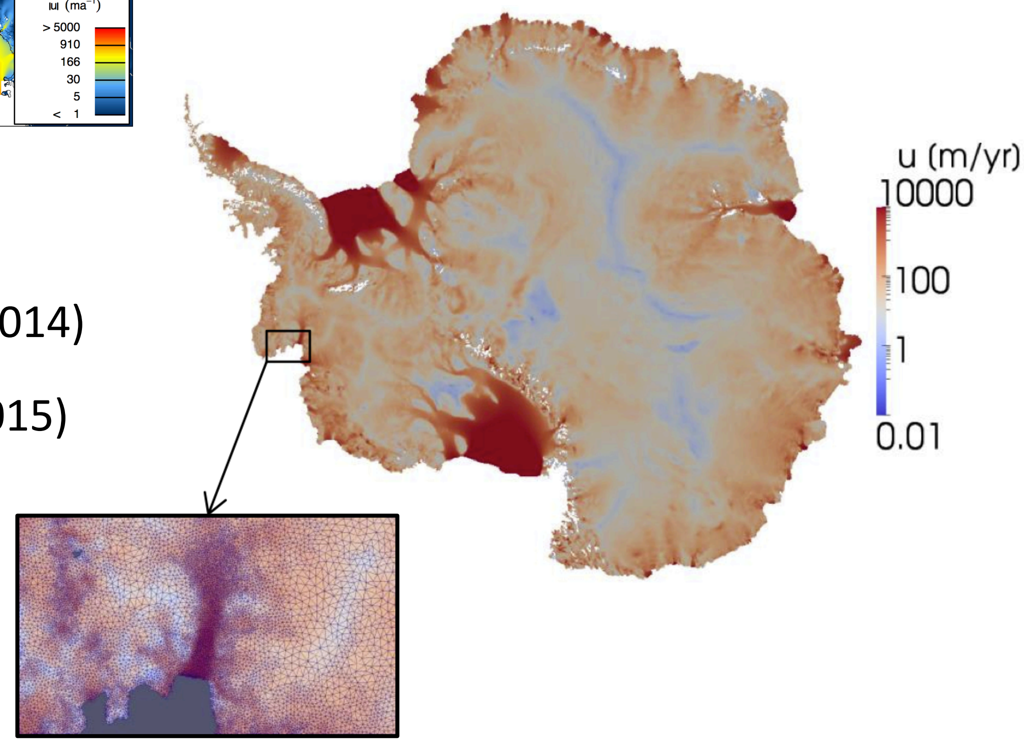
Zou et al., *Proc. CCGrid* (2015)

Gong et al. (2014) * BISICLES release *

Sun et al. (2014)

Wright et al. (2014)

Favier & Pattyn (2015)



Leng et al., *Comm. Comp. Phys.* (2014)

Perego et al., *J. Geophys. Earth Surf.* (2014)

Tezaur et al., *Geophys. Mod. Devel.* (2015)

Tezaur et al., *Proc. Comp. Sci.* (2015)

Zhang et al. *J. Glaciol.* (2015)

Motivation and Overview

Focus Area Updates

- **Verification & Validation**

Science Applications

Summary

Verification and Validation (V&V)

Verification of BISICLES and FELIX dycores using standard benchmarks and manufactured solutions (Tezaur et al., 2014; Leng et al., 2012) with nightly regression tests

Modeling frameworks tested with Land Ice Verif. And Valid. (LIVV) toolkit and pLIVV (“performance”) for tracking model performance during development (collaboration with SUPER)

Automated, nightly builds and testing for range of compilers & configurations using standard verification test cases

Supported on *Titan*, *Hopper* (*Edison* underway) and smaller devel. platforms (Mac, Linux clusters)

****** See poster by Evans et al. ******

Land Ice Verification and Validation (LIVV) Kit

Objective: Automated tool to evaluate ice sheet models
Release 1.0, https://github.com/LIVVkit/LIVVkit
July 15, 2015

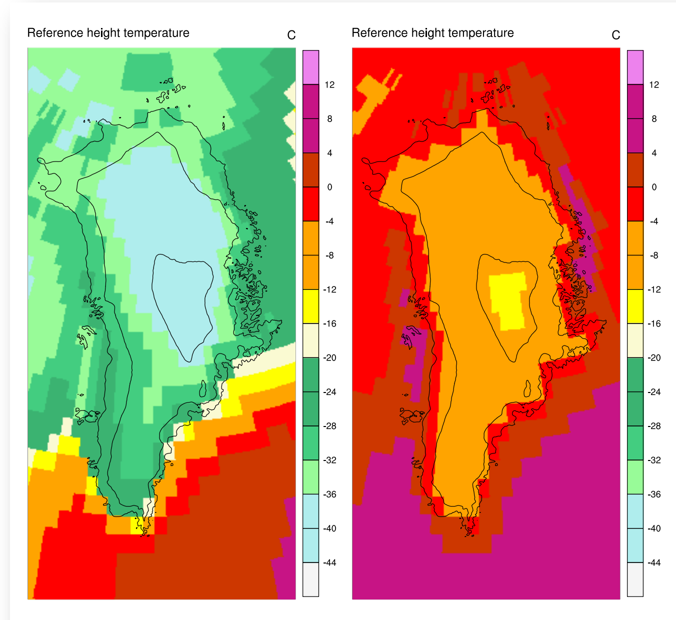
New Science:

- Provides comprehensive comparisons for a suite of benchmark tests of the CISM model
- Tested against the community ice sheet model on Titan, Hopper, Linux, and Mac platforms
- Generates suite of plots and test results on a hierarchical webpage

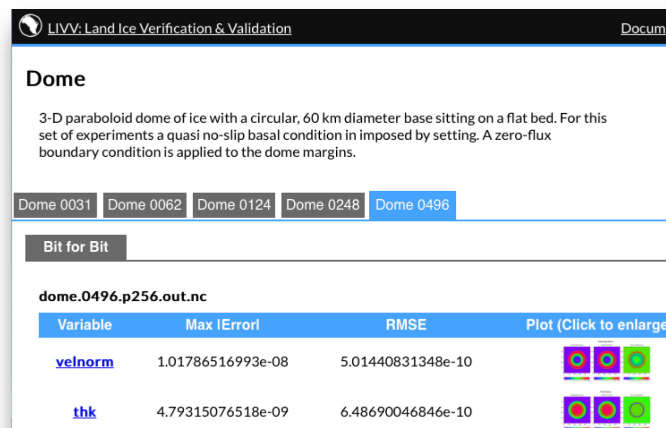
Significance

- Provides regression testing with full reproducibility information.
- Post-processing of solver and code performance for large problems detects performance changes and tests model 'value' of expensive new features; i.e. it provides a cost-benefit analysis of changes to code
- Provides hooks to add additional tests and dycore options.

Evans, Kennedy, Bennet, Worley (ORNL)

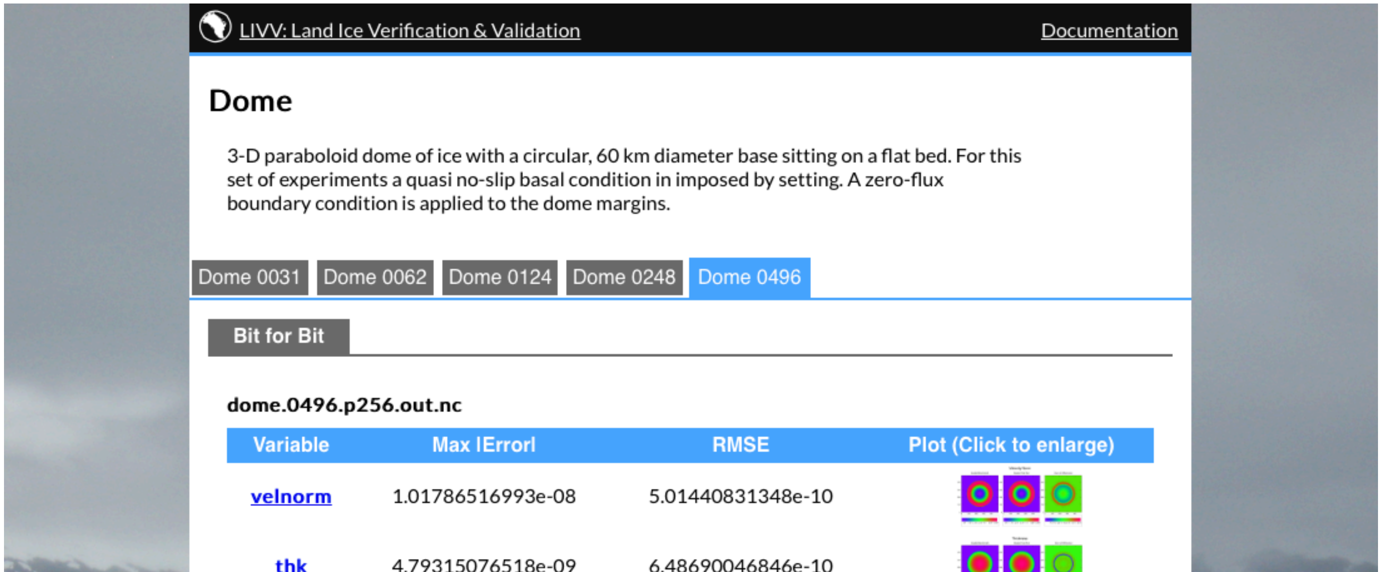


Example of test run data for validation from a coupled CESM 1.0 (pre-ACME) with active ice sheet model

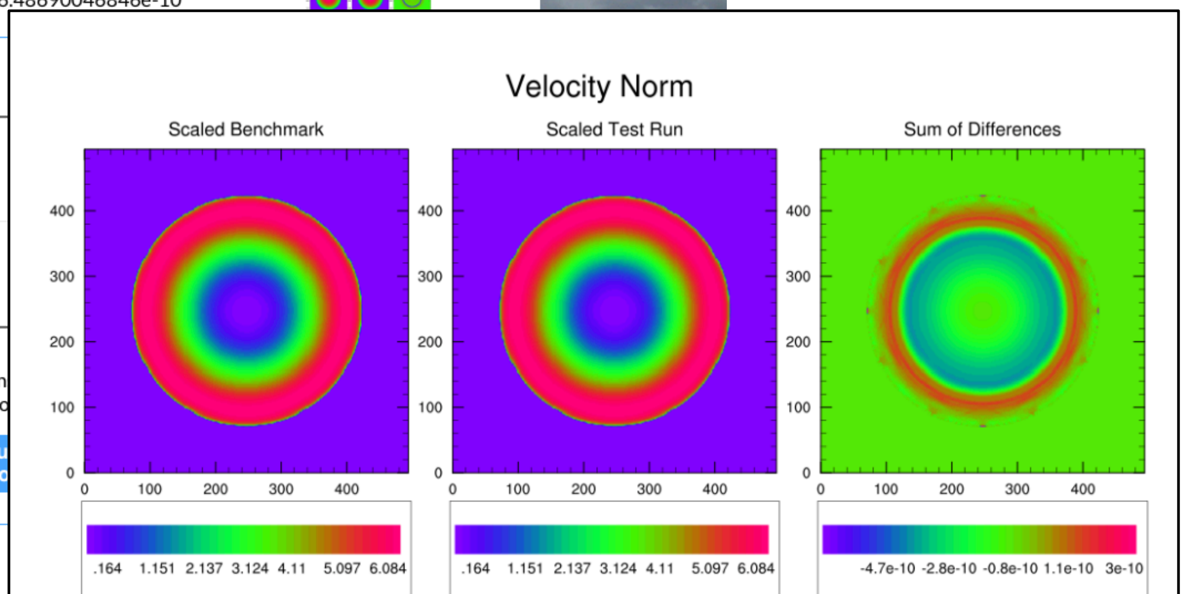


Verification test report (website screen shot)

Verification: LIVV



Report from recent ***LIVV*** test highlighting slight change in output for a standard test case



Evans, Kennedy, Bennet, Worley (ORNL)

Verification: pLIVV

LIVV: Land Ice Verification & Validation | Documentation

Verification Summary

	Std Out Files Parsed	Config File Matches	Bit for Bit
shelf			
Confined 0043	2	1/1	1/1
Circular 0041	2	1/1	1/1
dome			
Dome 0124	6	3/3	0/3
Dome 0496	2	1/1	0/1
Dome 0248	4	2/2	0/2
Dome 0062	4	2/2	0/2
Dome 0031	8	4/4	0/4
stream			
Stream 0025	2	1/1	0/1
ismip			
C 0020	2	1/1	1/1
C 0080	2	1/1	1/1
A 0080	2	1/1	1/1
F 0100	2	1/1	1/1
A 0020	2	1/1	1/1

Performance Summary

	Processor Counts	Avg. Runtime Change (% diff. from benchmark)
dome		
Dome 0124	001, 016, 256,	0.578956251919
Dome 0496	256,	1.53136376773
Dome 0248	064, 256,	0.900307583408
Dome 0062	001, 004,	-0.105990113333
Dome 0031	001, 002, 004, 008,	0.0467611972577

Validation Summary

No validation tests run

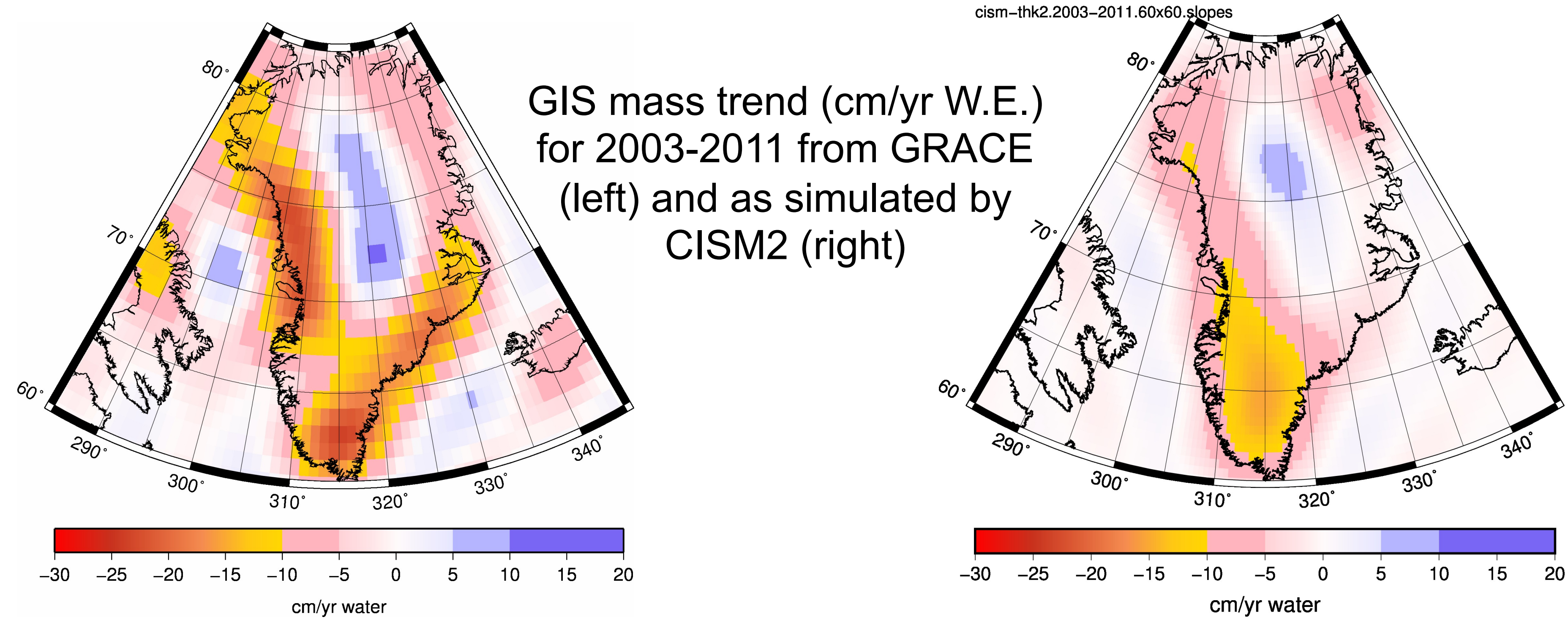
V&V Performed by kennedy at 07-13-2015 09:18:09

Report from recent ***pLIVV*** test highlighting slight change in performance on a standard test case

Evans, Kennedy, Bennet, Worley (ORNL)

(towards) Validation

- Metrics and validation: largely uncharted territory w.r.t. ice sheet models
- Validation: requires working with large, remote-sensing datasets, (unfunded) external collaborations (e.g., NASA), and non-DOE "domain science" expertise
- New and ongoing work:
  - "historical forcing" validation test cases for Greenland & Antarctica
  - Definition and implementation of metrics for validation of coupled simulations in ACME



GIS mass trend (cm/yr W.E.) for 2003-2011 from GRACE (left) and as simulated by CISM2 (right)

Price, Hoffman (LANL); Evans, Kennedy (ORNL); NASA-GSFC, Ohio State Univ., Univ. of S. Florida

Motivation and Overview

Focus Area Updates

Science Applications

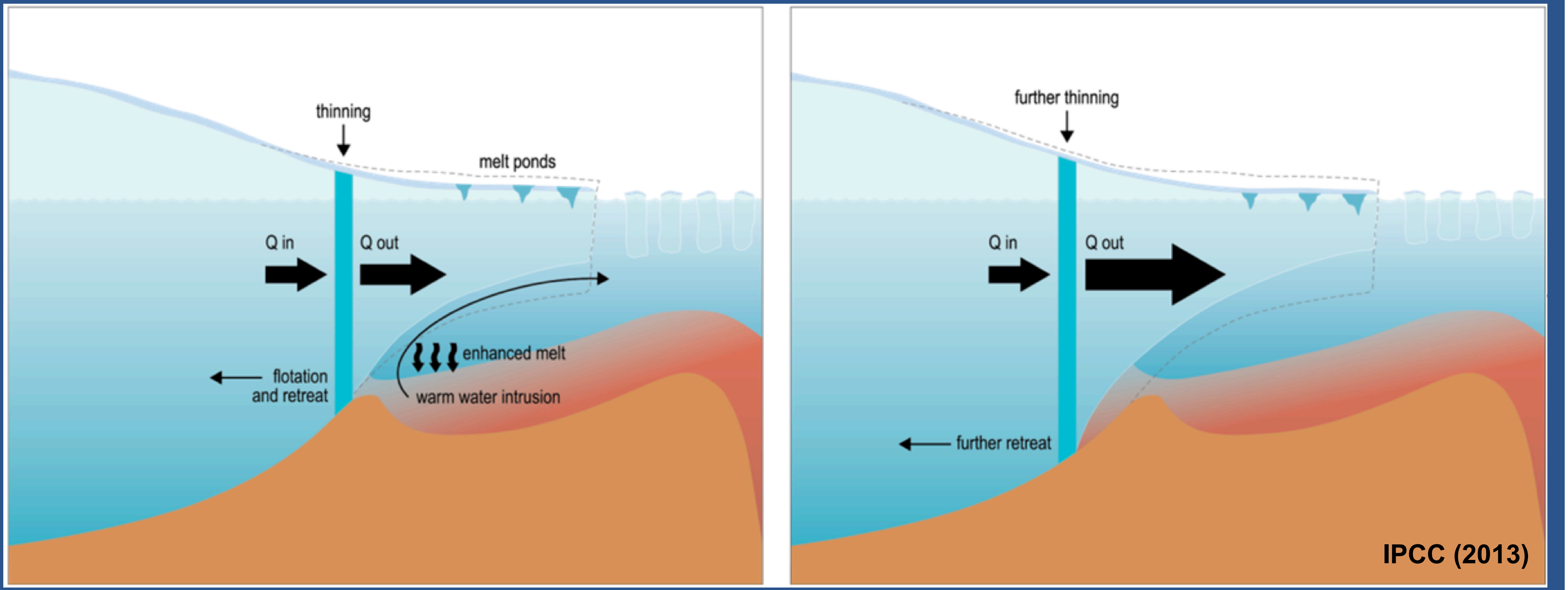
1. future SLR from Antarctica

Summary

Committed SLR from Antarctica

IPCC WG1 (2013): "*Based on current understanding, only the collapse of marine-based sectors of the Antarctic ice sheet, if initiated, could cause [SLR by 2100] substantially above the likely range [of ~0.5-1 m].*"

Committed SLR from Antarctica: Marine Ice Sheet Instability



Changes in ocean circulation mediate the contact between warm ocean waters and the ice sheet with impacts on submarine melting

Committed SLR from Antarctica

IPCC WG1 (2013): "*Based on current understanding, only the collapse of marine-based sectors of the Antarctic ice sheet, if initiated, could cause [21st century SLR] substantially above the likely range.*"

Paleorecord: partial Antarctic Ice Sheet (AIS) collapse occurred during past warm periods under CO_2 forcing similar to today

Present-day: strong evidence that ice sheet & ocean interactions are *the* mechanism responsible for retreat and increasing SLR from marine-based sectors of the AIS

Problem dependence on ice sheet & ocean interactions argues for an approach within a *coupled*, *ESM framework*

Support for Projecting Antarctic SLR in ACME

1) verification of ice sheet, ocean, and ice-ocean coupled models

2) early efforts at large-scale, coupled, Antarctic ice sheet and S. ocean simulations (POPSICLES)

3) semi-implicit geometry evolution methods (cannot allow ice sheet time step to be a bottleneck in coupled ESM)

Ice Sheet & Ocean Modeling: Idealized Experiments

MISMIP+ (3rd *Marine Ice-Sheet Model Intercomparison Project*)

- Ice-sheet only
- Parameterized basal melting
- **Goal: Test for accurate marine ice sheet dynamics**

ISOMIP+ (2nd *Ice shelf-Ocean Model Intercomparison Project*)

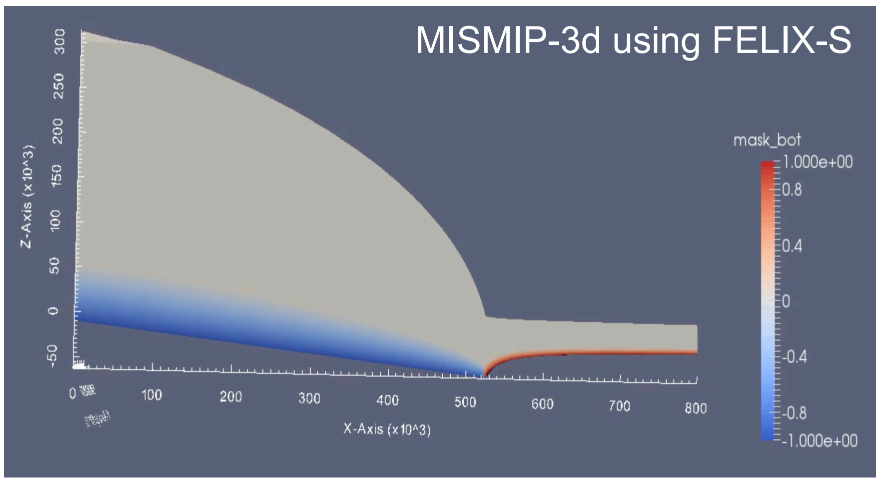
- Ocean only
- Ice topography from a MISMIP+ result
- **Goal: Test for accurate ocean dynamics near & beneath ice shelves**

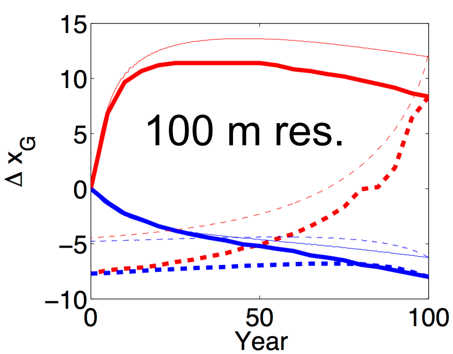
MISOMIP1 (1st *Marine Ice Sheet-Ocean Model Intercomparison Project*)

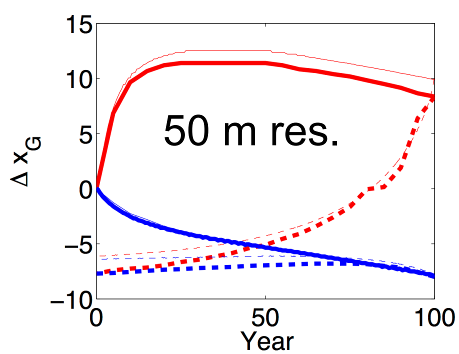
- coupling of MISMIP+ and ISOMIP+
- **Goal: Test dynamic ice sheet & ocean coupling**

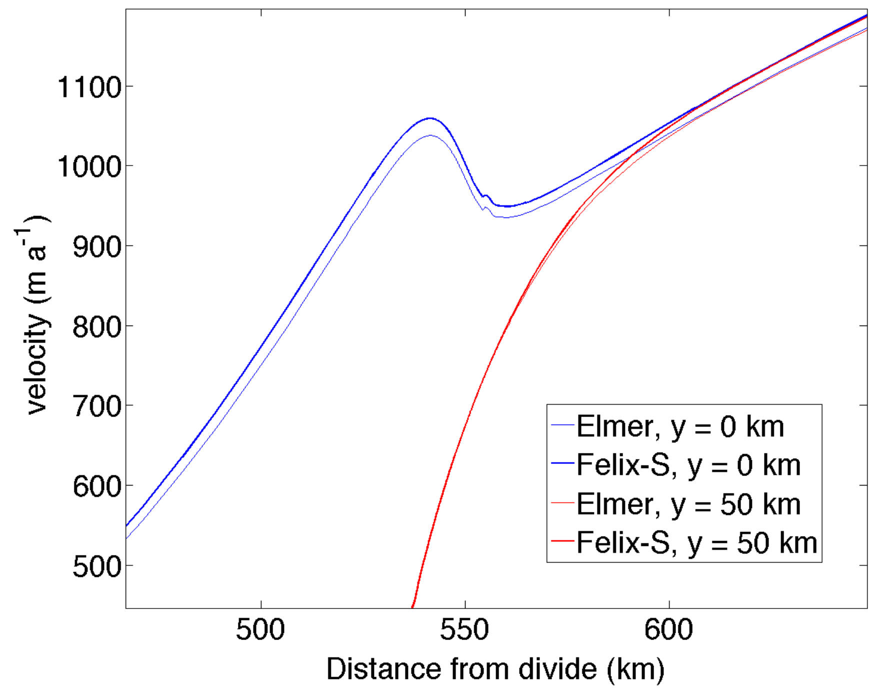
Validation of Marine Ice Sheet Dynamics With Felix-S

- High resolution Stokes model results taken as “truth” for idealized simulations of marine ice sheet dynamics (e.g., MISMIP*)
- To date, a single model is used by the international community
- We are doing 1:1 comparisons with that model to (1) provide additional confidence when benchmarking reduced order models against Stokes, and (2) to validate our own (DOE) marine ice sheet simulations







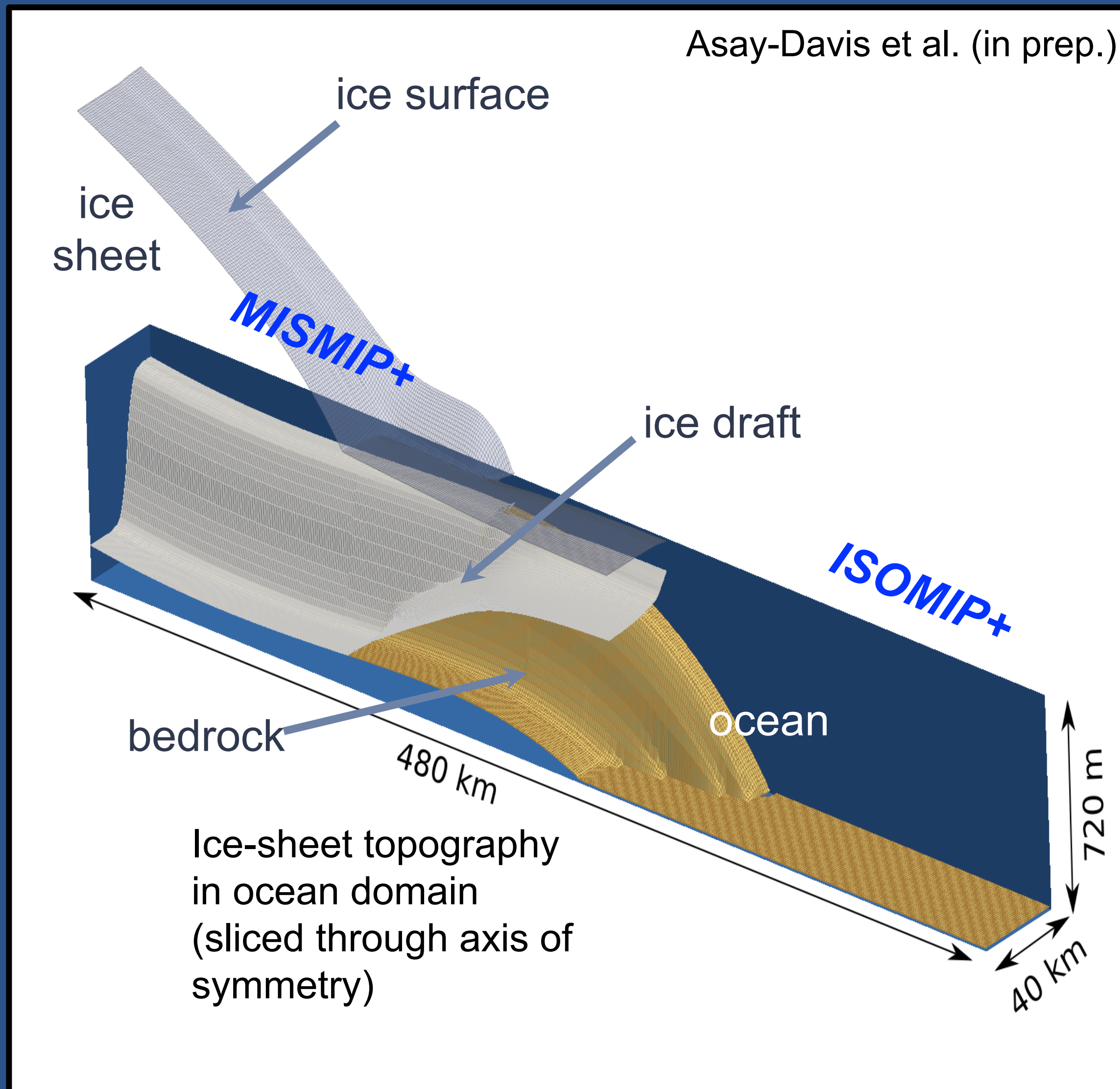


Zhang, Ju (USC); Gunzburger (FSU); Price (LANL)

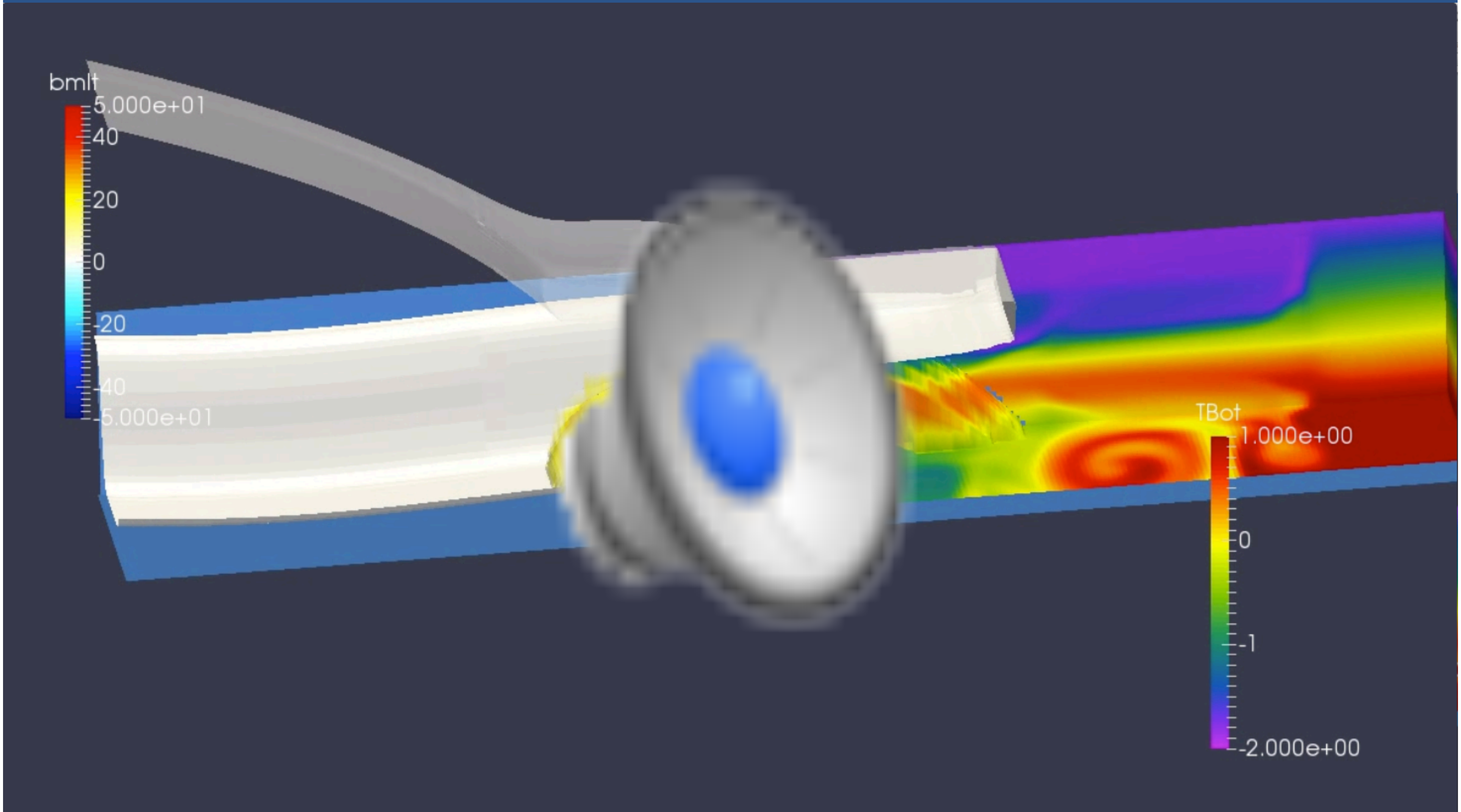
Ice Sheet & Ocean Modeling: Idealized Experiments

MISOMIP1 (1st *Marine Ice Sheet-Ocean Model Intercomparison Project*)

- coupling of MISMIP+ and ISOMIP+



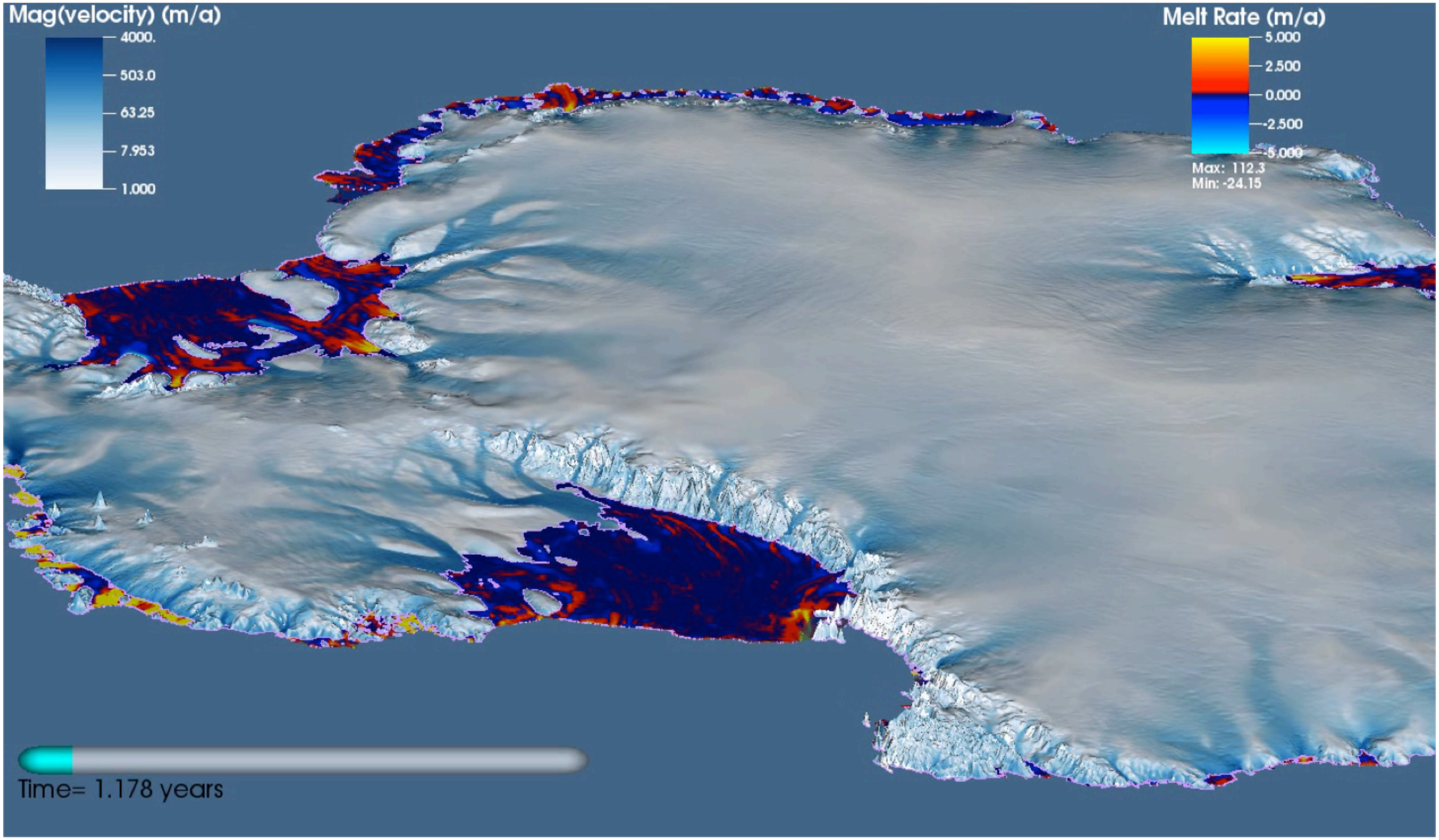
Ice Sheet & Ocean Coupling: MISOMIP with POPSICLES*



* POPSICLES = POP2x + BISICLES

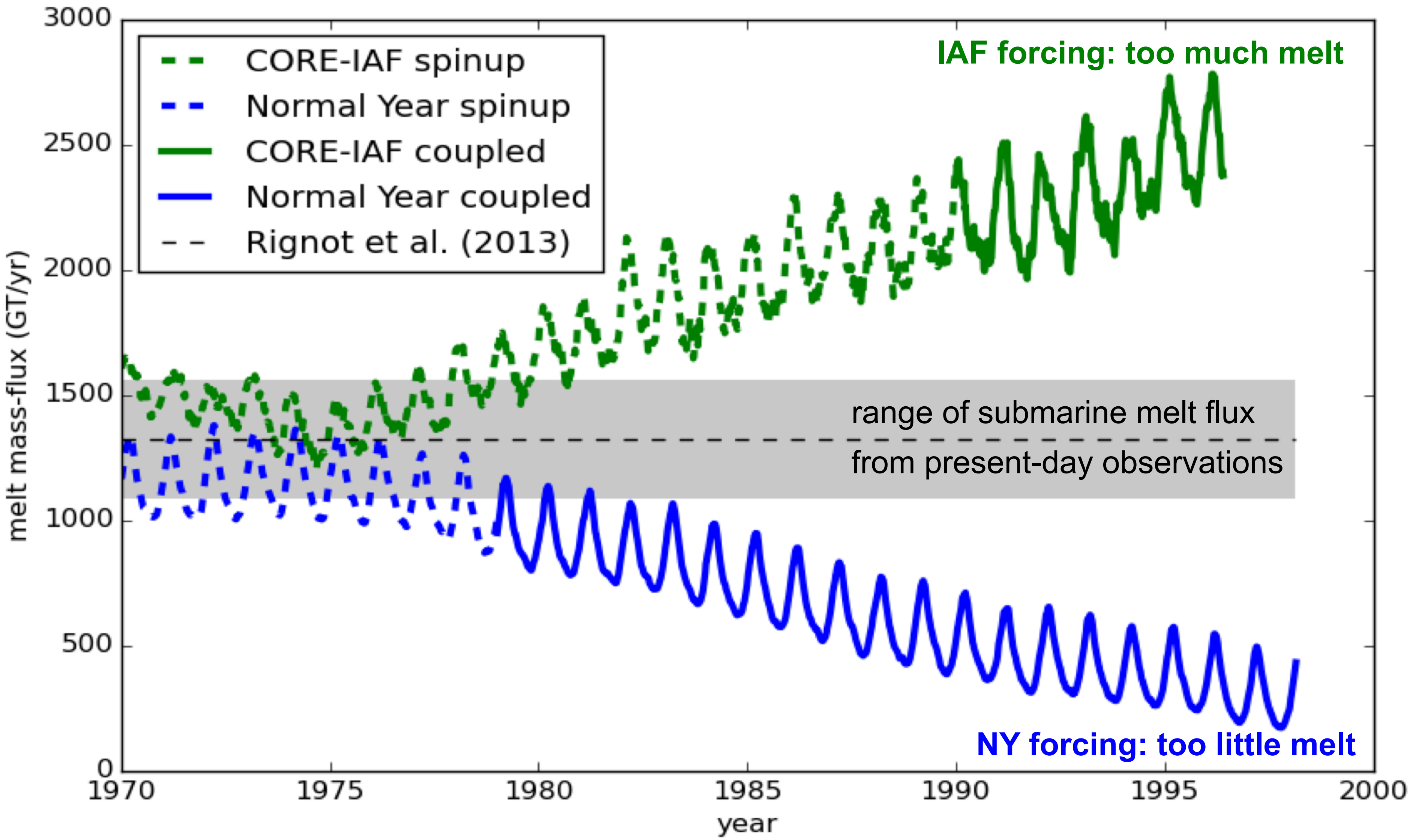
Asay-Davis (PIK) and Martin (LBNL)

POPSICLES: Coupled Antarctic Ice sheet & Southern Ocean Simulations



Asay-Davis (PIK) and Martin (LBNL)

*CORE-forced POPSICLES Simulations



*** CORE = standard atmospheric forcing dataset**

Asay-Davis (PIK) and Martin (LBNL)

POPSICLES Summary

Difficult to get ~SS initial condition with CORE forcing:

- NY too “cold” (not enough melt)
- IAF too “warm” (too much melt)

Cause - mixed-layer (ML) depth biases:

- NY: ML too deep, prohibits warm water access
- IAF: ML too shallow, to much warm water access

Recent advances:

- NY: anomalous high-salinity patches in forcing result in too much vertical mixing (bad forcing dataset?)
- IAF: adding vertical mixing param. should make ML depth more realistic (reasonable forcing dataset?)

Asay-Davis (PIK) and Martin (LBNL)

Semi-Implicit Methods for Thickness Evolution

Problem:

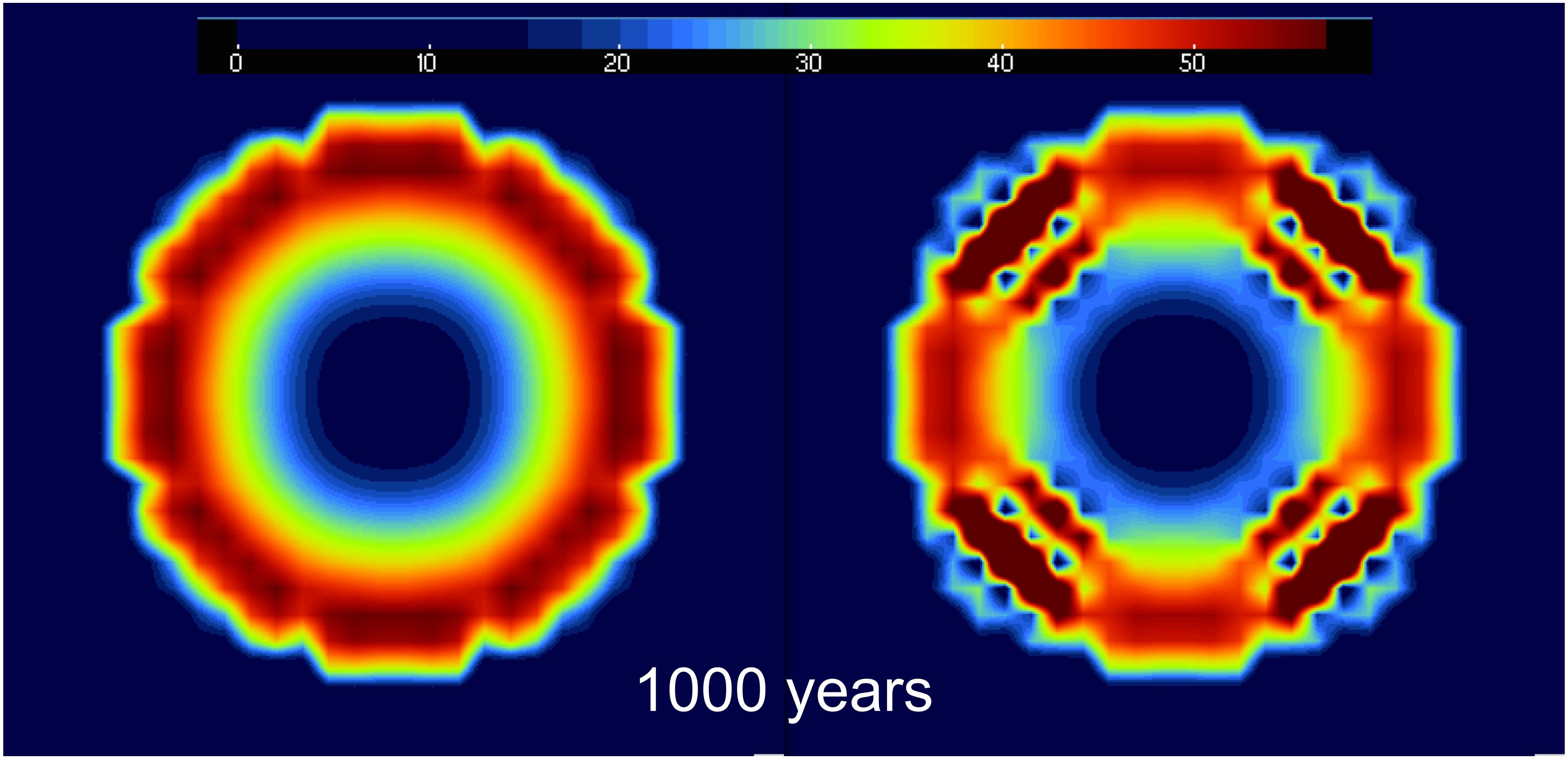
- explicit advection algorithms assume ice flow is hyperbolic
- ice flow can also be highly diffusive in areas
- stable time step for diffusion is generally << for advection
- ice sheet time step *cannot* be the bottleneck in ESM simulations

Practical Constraints:

- fully implicit methods are difficult to implement
- ice sheet modeling frameworks may be weakly coupled to momentum balance solvers (Fortran vs. C++ concerns)

Perego, Salinger (SNL); Price, Hoffman (LANL)

Thickness Evolution Instability:
Explicit Advection on Parabolic Dome



$dt = C * \tau_{diffussion}$ $dt = C * \tau_{advection}$

$0 < C \leq 1$

Semi-Implicit Methods for Thickness Evolution

Approach:

- The first-order Stokes momentum balance solved by *Felix-FO / Albany* includes ice thickness *only* as a RHS source term.
- In the velocity solver, iterate over time step to find velocity and thickness that are consistent
- Use this thickness as the forcing for the velocity solution
- Do all advection (including thickness) using this solution

$$\begin{cases} -\nabla \cdot \left(\mu \tilde{\mathbf{D}}\left(\mathbf{u}^{(n+1)}\right)\right) = -\rho g \nabla \left(b + H^{(n+1)}\right) & \text{in } \Omega_{H^n} \\ \nabla \cdot \mathbf{u}^{(n+1)} = 0 & \text{in } \Omega_{H^n} \end{cases} \qquad \frac{H^{(n+1)} - H^n}{\Delta t} + \nabla \cdot \left(\bar{\mathbf{u}}^{(n+1)} H^{(n+1)}\right) = \theta^n$$

Perego, Salinger (SNL); Price, Hoffman (LANL)

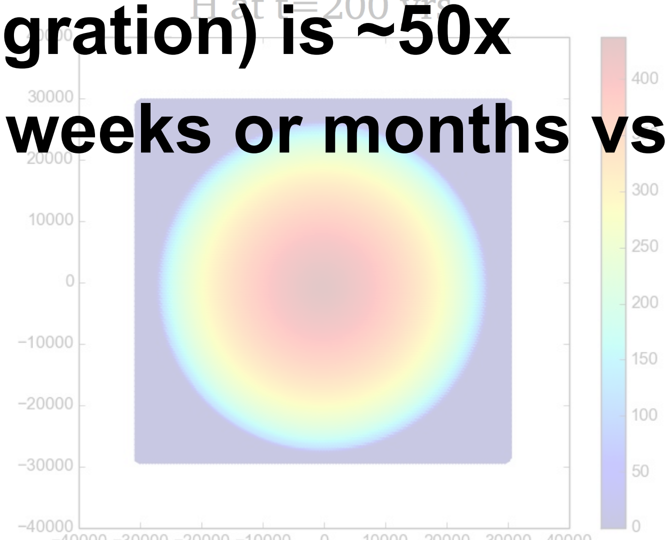
Semi-Implicit Methods for Thickness Evolution

Reference solution computed with sequential approach and time step of 5 months.

For realistic, moderate resolution Antarctic simulation:

- **cost per time step is ~3-4x explicit method**
- **speed-up (in time integration) is ~50x**
- **at hi-res: time step of weeks or months vs. hours**

Solution obtained with sequential coupling, **dt =1 yr**



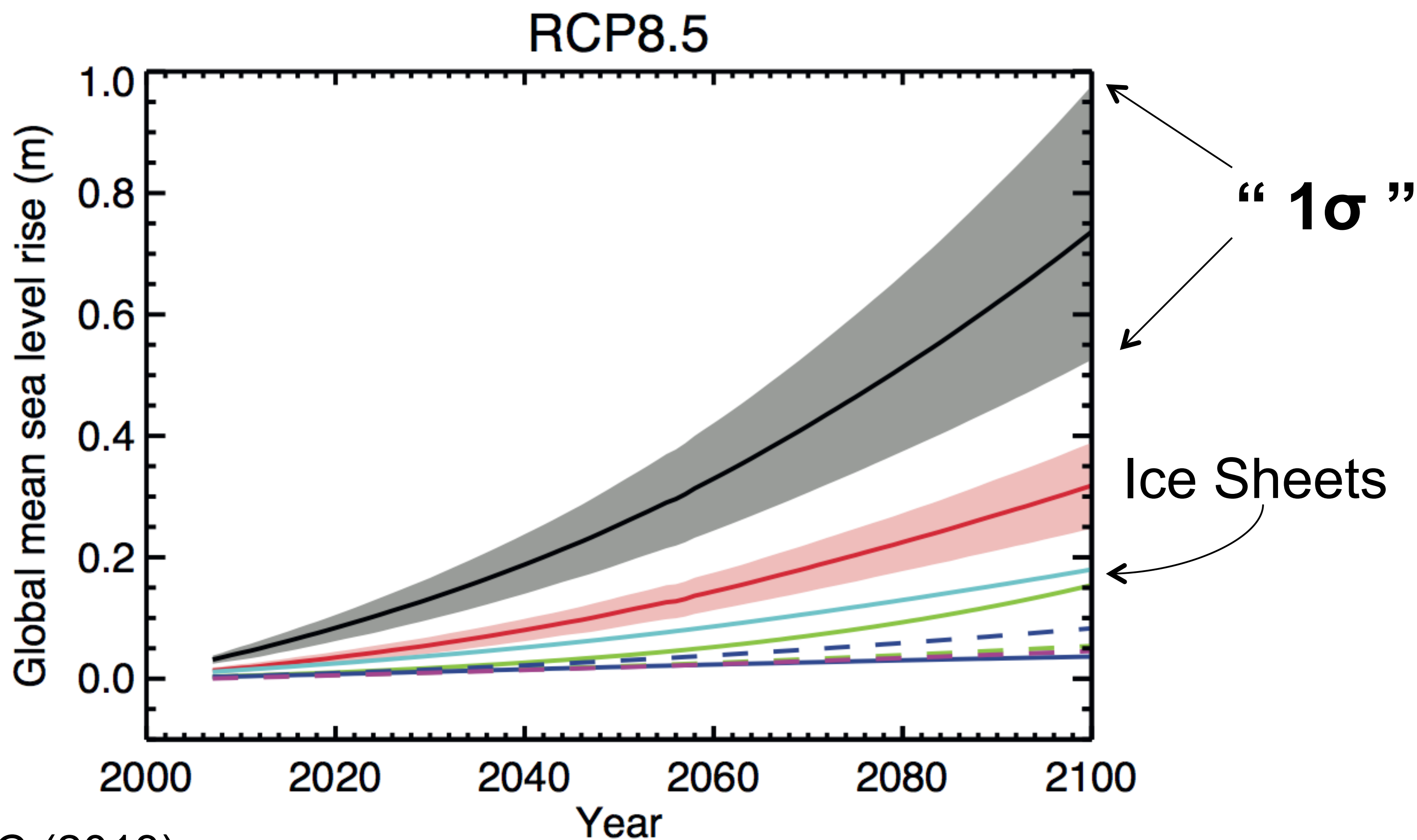
Solution obtained with implicit coupling, **dt=5 yrs**

Perego, Salinger (SNL);
Price, Hoffman (LANL)


Motivation and Overview
Focus Area Updates
Science Applications
2. Uncertainty in SLR from ice sheets
Summary

Quantification of Future SLR Uncertainty

For RCP8.5, [projected] global mean SLR for 2081–2100 (relative to 1986–2005) [is] 0.45–0.81 m … range at 2100 is 0.53–0.97 m



IPCC (2013)

Uncertainty Quantification

Uncertainty in predictions from ice sheet models come from:

(1) forcing uncertainties - related to uncertainties in future climate (explored through emissions-scenario-dependent and perturbed physics ensembles)

(2) model uncertainties – related to uncertainties in initial and boundary conditions (largely unexplored)

With the help of QUEST, PISCEES UQ is focusing primarily on the latter:

(i) Optimizing uncertain initial and boundary condition parameters

(ii) Estimating parameter uncertainties using a combination of intrusive (adjoint) and non-intrusive (sampling) approaches

(iii) Forward propagation of input parameter uncertainties to assign uncertainties to ice sheet model outputs of interest

***** *See poster by Jackson et al.* *****

UQ Workflow*: Proof of Concept

Q: How do uncertainties in the basal traction parameter β affect projections of sea level rise?

Data

Surface velocity $\mathrm{v} = \hat{\mathrm{v}} + \varepsilon_{\mathrm{v}}$

Surface elevation $h = \hat{h} + \varepsilon_h$

Bed topography $b = \hat{b} + \varepsilon_b$

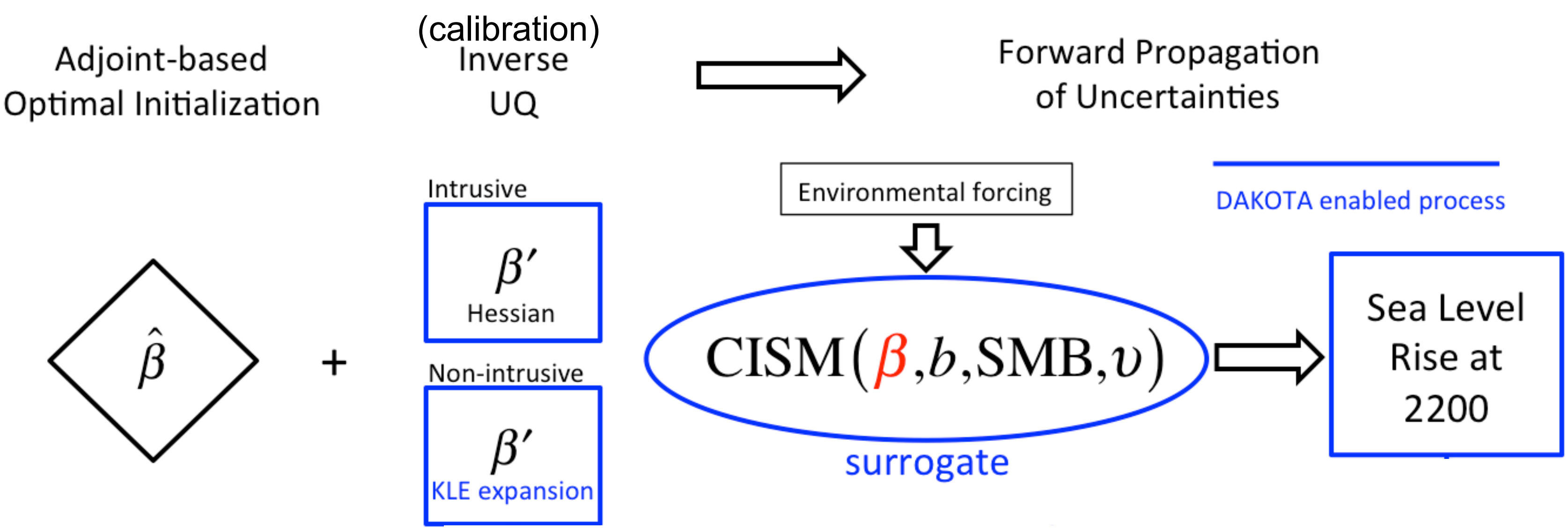
Uncertain parameters

basal traction $\beta = \hat{\beta} + \beta'$

MAP estimate

uncertainty

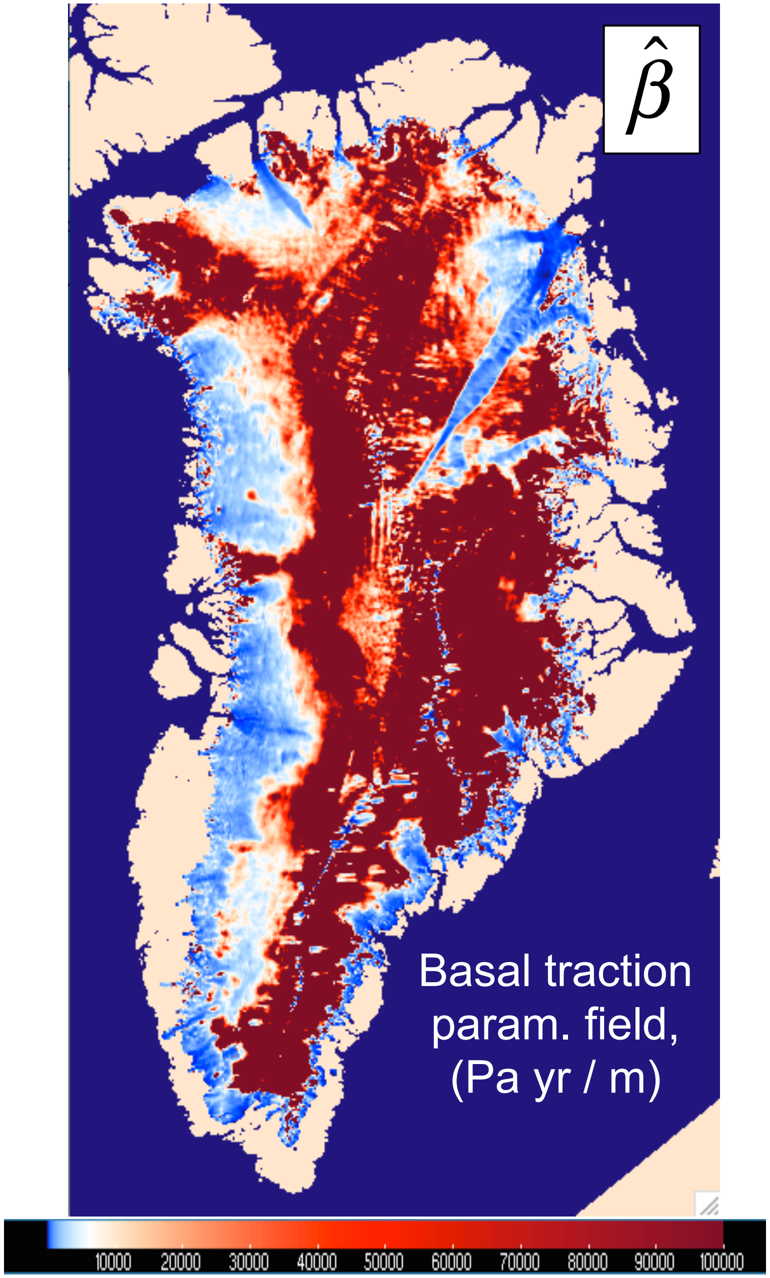
UQ Workflow

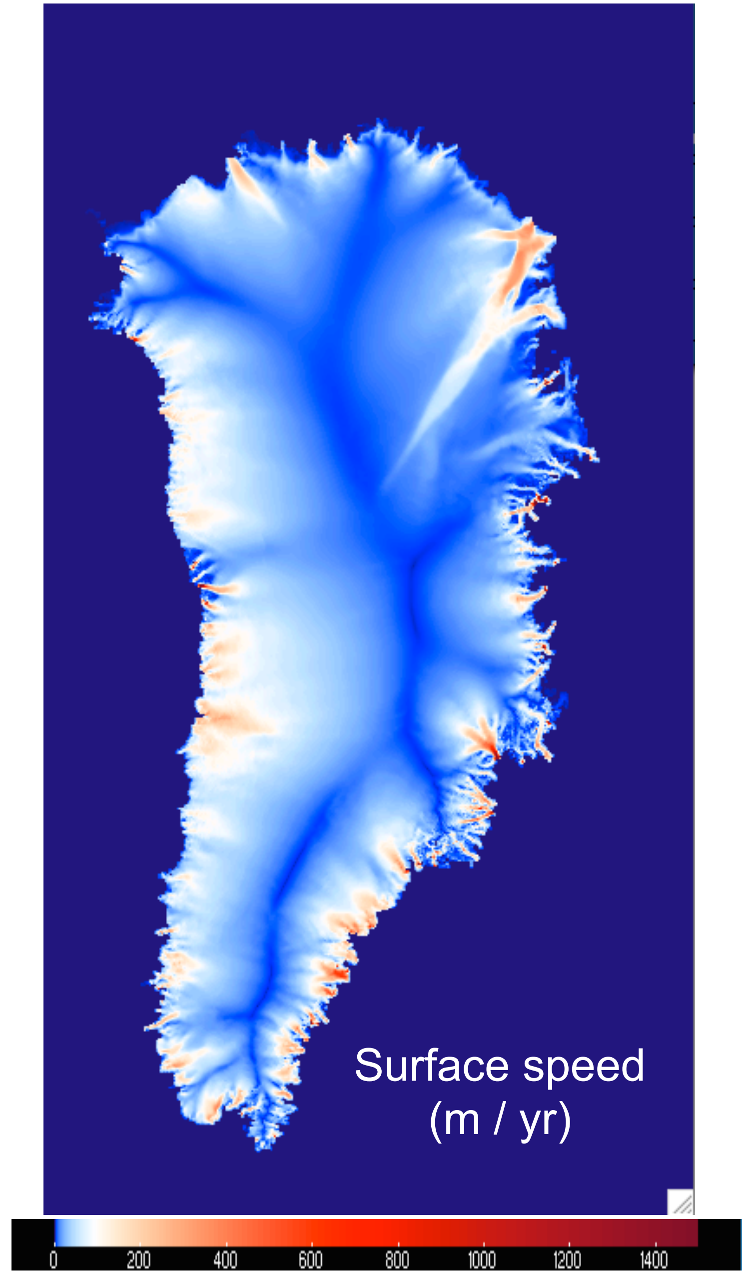


* *Heavily leveraging & building on previous work of Ghattas, Stadler, Petra, and Isaac*

Jackson, Heimbach (UT); Stadler (NYU); Tezaur, Salinger, Eldred, Jakeman (SNL); Price (LANL)

UQ Proof of Concept: Initial Conditions





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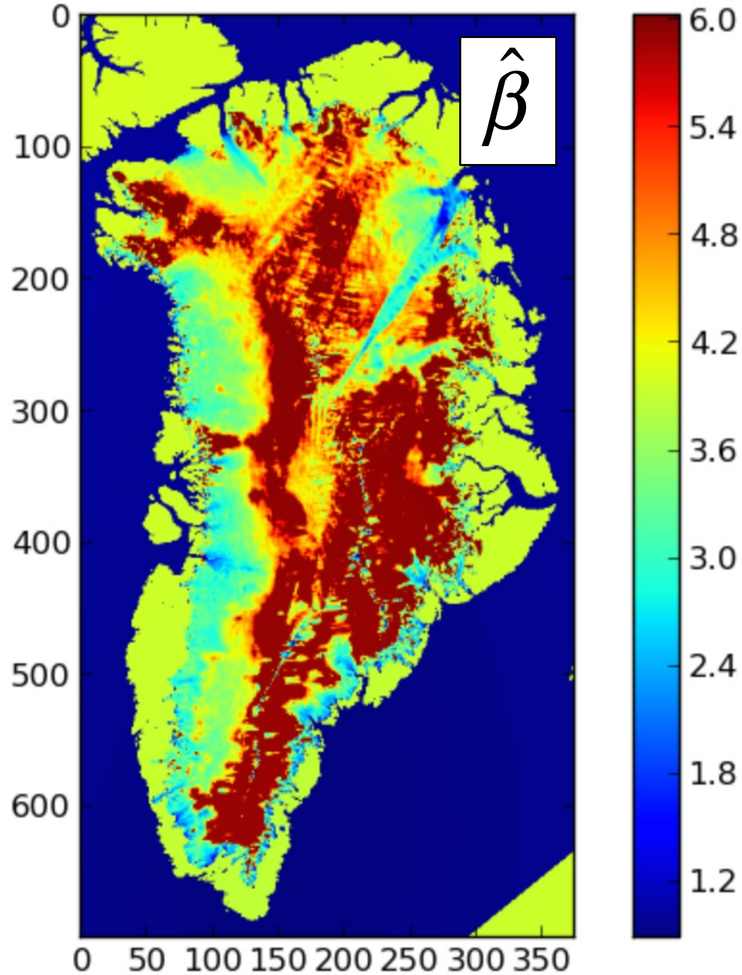
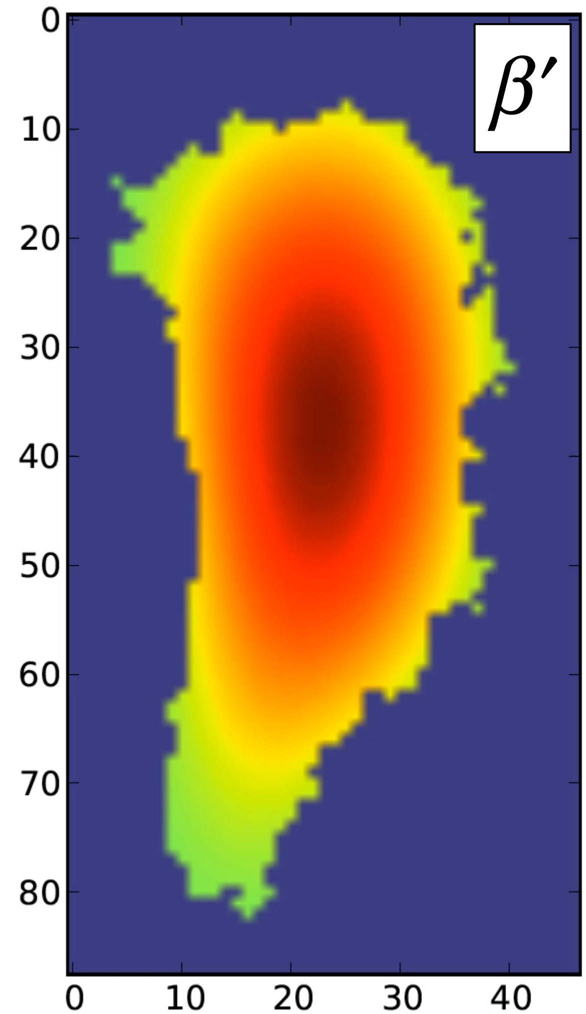
UQ Proof of Concept: Mean Field & Perturbations



Mean Field:
basal traction parameter
Log10(Pa yr/m)



Perturbation to Mean Field (structure)

$$\beta(\omega) = \bar{\beta} + \sum_{k=1}^{K} \sqrt{\lambda_k} \boldsymbol{\phi}_k \xi_k(\omega)$$

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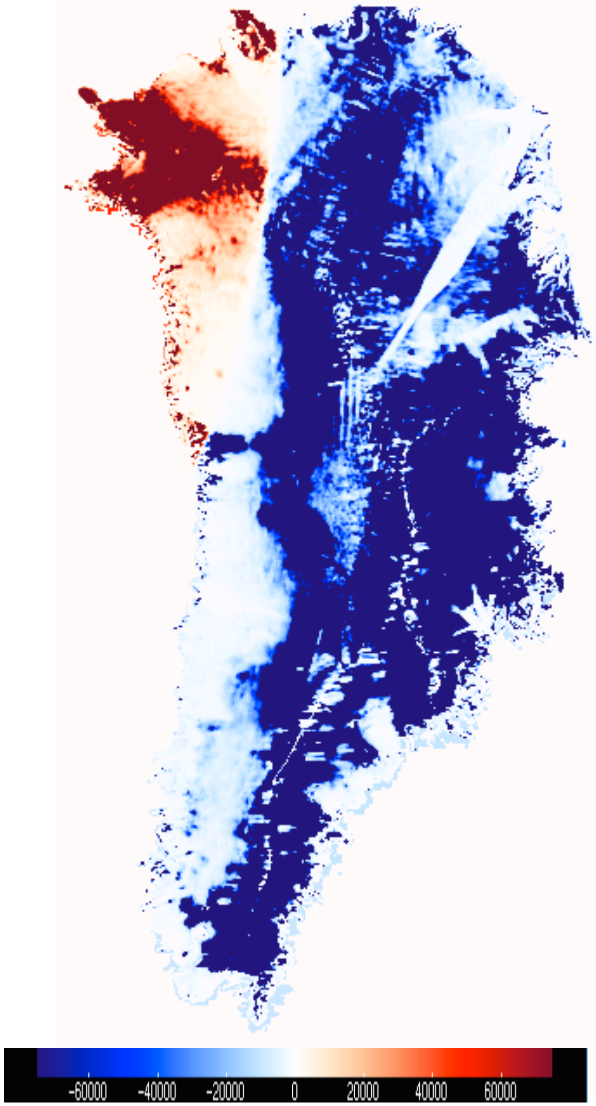
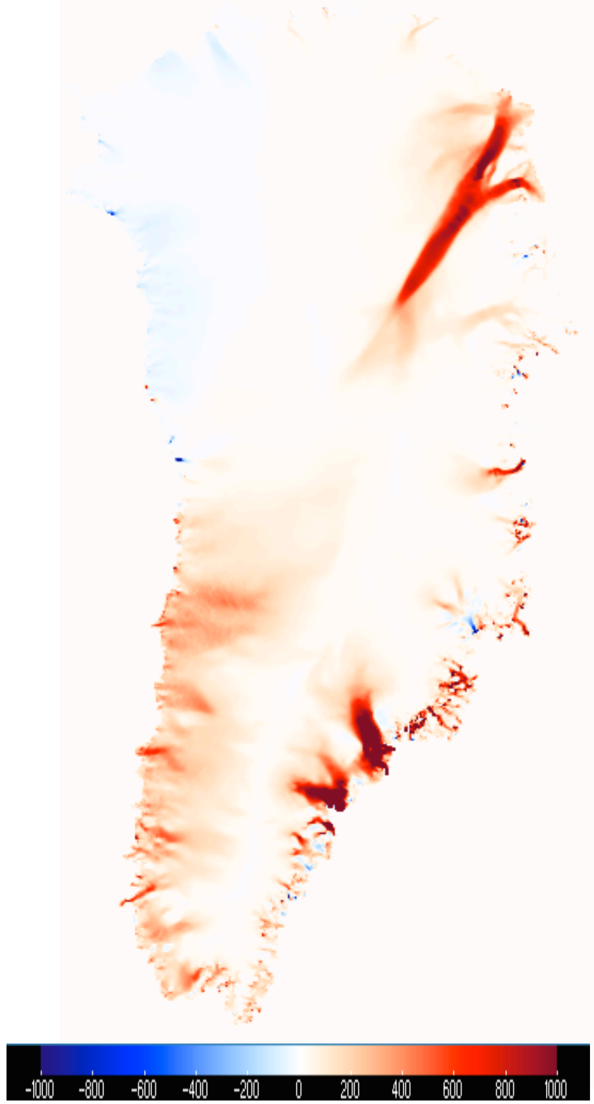
UQ Proof of Concept: Ensemble Member

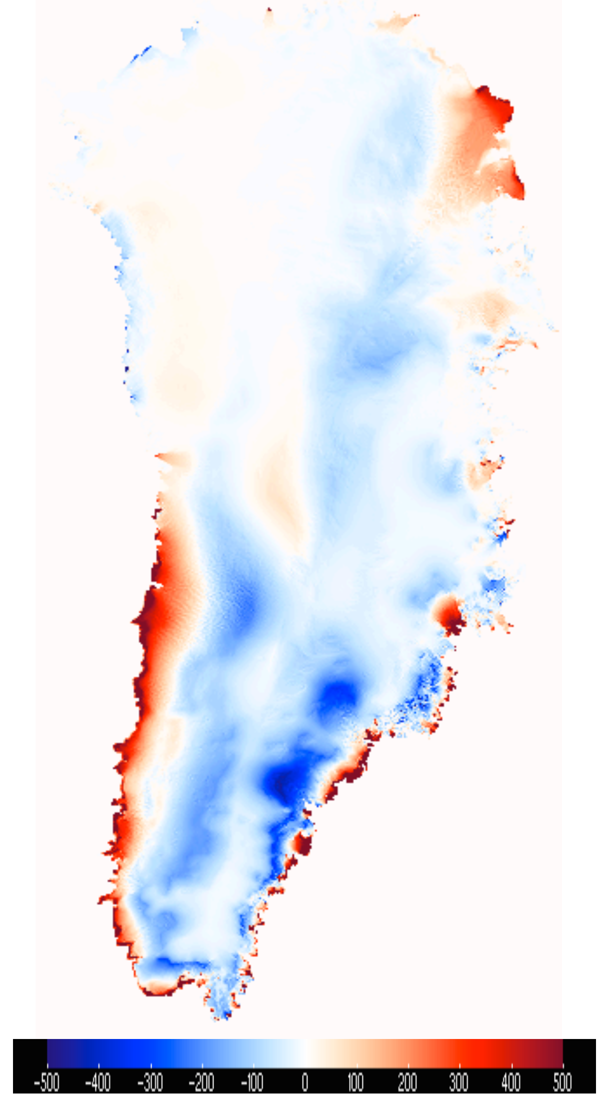
change in basal traction param. (Pa yr/m)



t=50 yrs: change in velocity (m/yr)



t=50 yrs: cumulative Thickness change (m)



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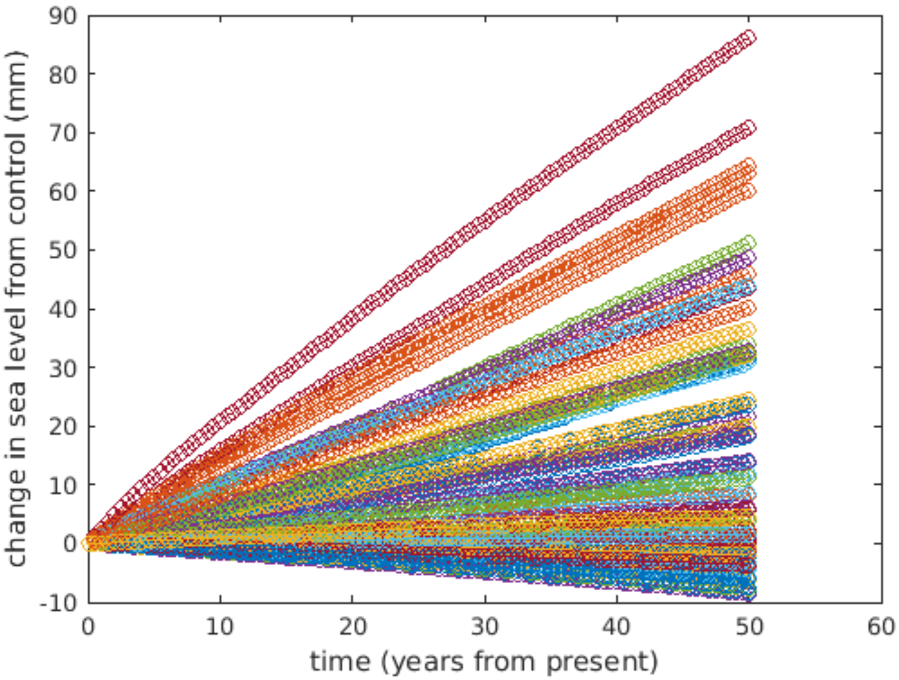
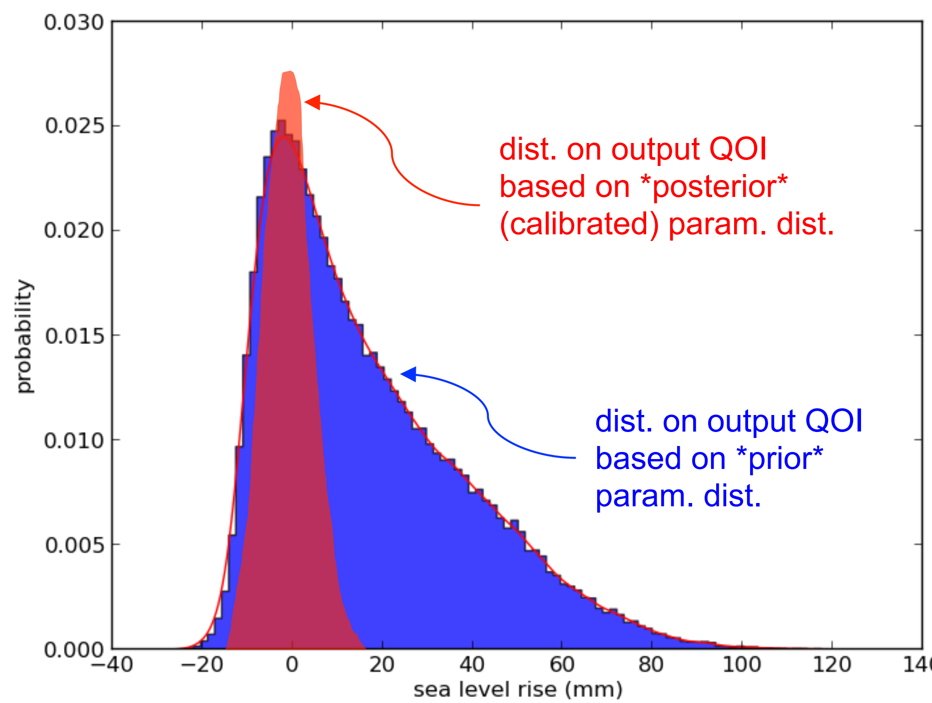
UQ Proof of Concept: Results



Left: Ensemble of sea-level change** simulated by CISM-Albany over 50 yrs from 66 forward model runs with perturbed basal sliding parameters. Perturbations from the "mean" field is based on a uniform distribution and 10 arbitrarily chosen KLE modes (proxies for structure in uncertainty)

** relative to a control run using mean field **

Right: Probability density function for cumulative sea-level change after 50 yrs, constructed from an emulator built using ensemble model outputs shown above (NOTE: this is the PDF based on the *prior* parameter uncertainty estimate)



Next Steps: use Hessian of cost function to characterize uncertainty structure (will require dimension reduction)

Motivation and Overview

Focus Area Updates

Science Applications

Summary

Summary

- mature ice sheet modeling frameworks (CISM and MPAS); robust & scalable dycores (BISICLES and FELIX)
- verification in place; V&V focus switching to validation
- ESM coupling and UQ efforts are integration points for dycore and V&V efforts, with current focus on …
- future sea-level rise from Antarctica
  - insight & experience gained from prelim. Effort
  - readying dycores & frameworks for use in ACME
- uncertainty in future sea-level rise from ice sheets
  - workflow “plumbing” is in place and tested
  - proof-of-concept for realistic, moderate scale problem
  - dimension reduction will be key to full realization

Summary

Interactions with SciDAC Institutes

FASTMath: *Chombo* AMR dycore and *Trilinos-Albany* unstructured mesh dycore allow for unprecedented, sub-km resolution, whole-Antarctic ice sheet simulations and advanced analysis, “UQ-ready” dycore, solving 10^9 unknowns on 16 k cpus

SUPER: optimal dynamical core settings for LCFs; performance instrumentation for dycores and FASTMath solver libraries (pLIVV); optimized communication-avoiding smoothers, ML and MG precond. Krylov methods for LCFs

QUEST: intrusive + non-intrusive *Dakota* and *Trilinos* based workflow for high-dimensional UQ using optimization tools for large-scale inversions, Bayesian calibration, and stochastic emulation, applied to idealized & realistic problems

SDAV: 6x acceleration of BISICLES iceberg detection algorithm

* = non-PISCEES collaborators

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Dycore Development & Performance

- **CISM:** M. Hoffman*, S. Price, W. Lipscomb (LANL)
  - **BISICLES**: D. Martin, E. Ng, S. Williams (LBNL)

- **MPAS-LI:** M. Hoffman*, S. Price, W. Lipscomb (LANL)
  - **FELIX-FO:** I. Tezaur, M. Perego, A. Salinger, R. Tuminaro (SNL)
  - **FELIX-S:** M. Gunzburger (FSU), L. Ju & T. Zhang (USC)

- **Performance:** R. Tuminaro (SNL), S. Williams (LBNL), P. Worley (ORNL)

V & V: K. Evans, M. Norman, P. Worley, J. Kennedy, A. Bennet (ORNL)

UQ: M. Eldred, J. Jakeman, A. Salinger (SNL); C. Jackson, O. Ghattas (UT Austin); P. Heimback (MIT, UT Austin); G. Stadler (NYU)

ESM Integration: J. Fyke* (LANL); W. Sacks, M. Vertenstein (NCAR)

POP2x and MPAS Ocean Models: X. Asay-Davis* (PIK); M. Petersen*, D. Jacobsen*, T. Ringler* (LANL)